Dynamic Statistical Scaling in the Landau-de Gennes Theory of Nematic Liquid Crystals

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Abstract

In this article, we investigate the asymptotic behaviour of a correlation function associated with a nematic liquid crystal system undergoing an isotropic-nematic phase transition following an instantaneous change of system temperature. Within the setting of Landau-de Gennes theory, we confirm a hypothesis in the condensed matter physics literature on the average self-similar behaviour of the correlation function in the asymptotic regime at time infinity, namely

$$\left\| c_{\mu_0}(r,t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3,\, dr)} = \mathcal{O}(t^{-\frac{1}{2}}) \quad \text{as} \quad t \longrightarrow \infty,$$

where the correlation function $c_{\mu_0} : \mathbb{R}^3 \times (0,\infty) \to \mathbb{R}$ is defined by (6) below. In the final sections, we also pass comment on other possible scaling behaviour of the correlation function.

1. Introduction

Nematic liquid crystals form a class of condensed matter systems whose constituent rod-like molecules give rise to rich macroscopic nonlinear phenomena. Thermotropic nematic liquid crystals are a well-studied subclass of nematics whose physical properties change dramatically with variation of system temperature. It is commonly observed in the laboratory that above a certain temperature threshold, the rod-like molecules exhibit no local orientation preference, which is known widely as the *isotropic phase* of the material. Yet, reducing the temperature of the material below this threshold results in the molecules arranging themselves along locally preferred directions, yielding the so-called *nematic phase*.

Models for the dynamics of this transition from isotropy to a nematic phase in liquid crystals present many challenging mathematical questions, both in continuum theories and also in statistical mechanics. In the laboratory, the transition between the isotropic and nematic phases is observed to be effected by the seeding and subsequent growth of nematic 'islands' in the ambient isotropic phase. The characteristic length scale $L \equiv L(t)$ of these structures increases with time once the system is coerced into a transition of phase. It is argued in the physics literature that the domain coarsening of

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the nematic phase is a scaling phenomenon, namely the *structure* of the nematic profile at late times looks *statistically self-similar* to those profiles at an earlier time, up to a simple rescaling in space. We invite the reader to consult the extensive review article of Bray [4] for a helpful introduction to this area of condensed matter physics. Laboratory experiments performed by Pargellis et al. [16], in which a nematic liquid crystal system was contrived to resemble a dynamic XY-model, support this argument.

It is the aim of this paper to articulate such behaviour of thermotropic nematic systems in a mathematically rigorous manner. We work within the framework of continuum PDE theory, as opposed to the forbidding setting of statistical mechanics.

As the isotropic-to-nematic phase transition is inherently dynamic, we require an appropriate evolution equation to model this coarsening phenomenon. The model we employ in this paper is the L^2-gradient flow of the well-studied Landau-de Gennes energy. This energy is given by

$$E_{\mathrm{LdG}}[Q] := \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla Q|^2 + \frac{a(\theta)}{2}\mathrm{tr}\left[Q^2\right] - \frac{b}{3}\mathrm{tr}\left[Q^3\right] + \frac{c}{4}\left(\mathrm{tr}\left[Q^2\right]\right)^2 \right) dx \tag{1}$$

for appropriately regular maps Q, the gradient flow of which is

$$\frac{\partial Q}{\partial t} = \Delta Q - a(\theta)\, Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left[Q^2\right] I \right) - c\,\mathrm{tr}\left[Q^2\right] Q. \tag{2}$$

We invite the reader to consult the works of Ball and Zarnescu [2], Ball and Majumdar [3], Majumdar and Zarnescu [13] and Nguyen and Zarnescu [15] for an introduction to analytical and topological aspects of Landau-de Gennes theory.

In order to achieve our goal, we must first state in precise quantitative terms what we mean by *structure* of nematic profiles and also by *statistical self-similarity*. Indeed, both of these concepts lead us naturally to the mathematical problem of obtaining a phase portrait for a quantity (a correlation function) describing the average behaviour of solutions of the gradient flow of (1) above. We argue that one might view this as a convenient simplification of the infinite-dimensional dynamics generated by this PDE on its natural phase space, which captures the essential qualitative behaviour of solutions. However, antecedent to both of these ideas is the notion of *order parameter*, which we now discuss in section 1.1 before introducing correlation functions in section 1.2 (related to structure) and statistical solutions of PDEs in section 1.3 (related to statistical self-similarity).

1.1. **The de Gennes Q-tensor Order Parameter.** The first task when building a continuum model of such phase transition phenomena is to decide upon an appropriate order parameter that captures small scale material structure and allows one to distinguish between different phases of the material under study. In this article, we work with the Q-tensor order parameter which is able to describe both uniaxial and biaxial phases of nematic liquid crystals, as opposed to, say, the director-field formalism of Ericksen-Leslie theory [11] or Oseen-Frank theory [9].

Let us suppose that to each point x in a material domain $\Omega \subseteq \mathbb{R}^3$ we associate a probability density function ρ_x on molecular orientations which lie in $\mathbb{S}^2$. In order to

model the $\mathbb{Z}_2$ head-to-tail symmetry of nematic molecules, each density is endowed with the antipodal symmetry $\rho_x(n) = \rho_x(-n)$ for all $n \in \mathbb{S}^2$. It was the idea of the Nobel prize-winning physicist Pierre-Gilles de Gennes that one might consider the essential macroscopic information of the system to be contained in the matrix of second moments of ρ_x with respect to molecular orientations. The *de Gennes Q-tensor order parameter* (with respect to the density ρ_x) is defined to be

$$Q(x) := \int_{\mathbb{S}^2} \left(n \otimes n - \frac{1}{3} I \right) \rho_x(n)\, dn. \tag{3}$$

It is a normalised matrix of second moments of ρ_x, and one may quickly check that $Q(x)$ is a traceless and symmetric 3×3 matrix.

At the level of probability measures on molecular orientations, the uniform density $\overline{\rho} = 1/|\mathbb{S}^2|$ corresponds to the isotropic phase of nematics. It is important to note that the term $-1/3I$ (which contains no information about the system) is included in the above definition (3) of the Q-tensor by convention, so as to render Q identically zero in the isotropic phase. The Q-tensor may then be thought of as a macroscopic order parameter that measures the deviation of the system from isotropy. For a more detailed introduction to the Q-tensor order parameter, one might wish to consult de Gennes and Prost [5], Majumdar [12] or Newton and Mottram [14].

We denote the order parameter manifold of all such matrices by $\mathrm{Sym}_0(3)$, namely

$$\mathrm{Sym}_0(3) := \left\{ Q \in \mathbb{R}^{3\times 3} \, : \, Q^T = Q \quad \text{and} \quad \mathrm{tr}[Q] = 0 \right\},$$

where $\mathrm{tr} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ denotes the familar matrix trace operator. We subsequently refer to maps which take their values in $\mathrm{Sym}_0(3)$ as nematic profiles.

1.2. **'Structure' of Nematic Profiles: Correlation Functions.** The measure of structure of nematic profiles $Q : \mathbb{R}^3 \times (0,\infty) \to \mathrm{Sym}_0(3)$ we employ in this paper is the two-point spatial correlation function $c : \mathbb{R}^3 \times (0,\infty) \to \mathbb{R}$ defined by

$$c(r,t) := \frac{\displaystyle\int_{\mathbb{R}^3} \mathrm{tr}\left[Q(x+r,t) Q(x,t) \right] \, dx}{\displaystyle\int_{\mathbb{R}^3} \mathrm{tr}\left[Q(x,t)^2 \right] \, dx}.$$

One may think of c as quantifying how correlated different regions of a nematic profile are with one another and thus as some measure of the spatial structure of the system as it evolves over time. For further information on the use of correlation functions in condensed matter physics, we recommend that the reader consult Sethna ([19], Chapter 10).

As mentioned above, it is argued in the physics literature (see for instance Denniston et al. [6] or Zapotocky et al. [21]) that once a system is coerced into an isotropic-nematic phase transition the correlation function assumes a self-similar form asymptotically in time. In summary,

$$\langle c(r,t) \rangle \sim \Gamma\left(\frac{r}{L(t)} \right) \quad \text{in an appropriate topology as} \quad t \longrightarrow \infty, \tag{4}$$

where Γ is some 'universal' scaling function and $L(t)$ is the aforementioned characteristic length scale of nematic domains which invade the isotropic phase. The angular brackets $\langle\cdot\rangle$ signify that one considers a suitable average value of the correlation function as computed over many repeated experimental trials, smoothing out anomalous data gathered from experiment. If one then wishes information on the structure of this system for large values of time t, one need only rescale in the spatial variable r.

In order to model such an averaging procedure in a mathematically rigorous manner, we employ the notion of statistical solution of evolution equations introduced by Foiaş [7] and also by Vishik and Fursikov [10]. This notion of solution to nonlinear PDE was subsequently studied many authors in the mathematical theory of the Navier-Stokes equations to explore aspects of turbulence theory. We now outline the significance of statistical solutions in our study of phase transitions.

1.3. **'Statistical Self-similarity': Statistical Solutions of PDEs.** One can show that the semiflow $\{S(t)\}_{t\geq 0}$ of the gradient flow (2) of E_{LdG} possesses neither a global attractor nor an inertial manifold in the natural phase space $H := L^2(\mathbb{R}^3)\cap L^6(\mathbb{R}^3)$, which is unfortunate as both objects are well suited to revealing asymptotic structure of dynamics. Since we are interested in studying the time asymptotics of the correlation function c_{μ_0}, this presents a significant challenge. Thus, acknowledging the structure of the manifold of solution trajectories

$$\mathcal{M} := \bigcup_{Q_0\in H}\left\{\{Q(\cdot,t)\}_{t\geq 0}\,:\,Q(\cdot,0)=S(0)Q_0=Q_0\right\},$$

as being rather complicated, we ask naïvely what one could say if one turns instead to the manifold of measure-valued statistical solutions

$$\mathcal{N} := \bigcup_{\mu_0\in\mathsf{M}_0(H)}\left\{\{\mu_t\}_{t\geq 0}\,:\,\mu_t|_{t=0}=\mu_0\right\}, \tag{5}$$

where $\mathsf{M}_0(H)$ denotes the set of all Borel probability measures on H. The manifold $\mathcal{N}$ is 'coarser' than $\mathcal{M}$ in terms of information, in the sense that each such statistical solution μ_t of (2) at time t is insensitive to changes on sets of measure 0. In order to make use of this insensitivity to 'fine structure' of the trajectory manifold $\mathcal{M}$, and to perhaps also give us hope of characterising one qualitative aspect of solutions of (2) on H (section 6), we redefine the correlation function c as

$$c_{\mu_0}(r,t) := \frac{\displaystyle\int_H\int_{\mathbb{R}^3}\mathrm{tr}\left[Q(x+r)Q(x)\right]\,dx d\mu_t(Q)}{\displaystyle\int_H\int_{\mathbb{R}^3}\mathrm{tr}\left[Q(x)^2\right]\,dx d\mu_t(Q)}. \tag{6}$$

It is with this definition of the correlation function we work throughout this paper, as opposed to the earlier-given definition (4) which is supported only on single trajectories in $\mathcal{M}$. Moreover, it allows us to give good mathematical sense to the average $\langle\cdot\rangle$ discussed above, namely $\langle c(r,t)\rangle := c_{\mu_0}(r,t)$.

The gradient flow (2) takes the shape of a nonlinear heat equation for the evolution of nematic profiles Q. As this equation generates a strongly-continuous semigroup of

solution operators $\{S(t)\}_{t\geq 0}$ on phase space H, it is possible to deal more concretely with the evolution of initial measures as opposed to the 'Liouville equation' formalism[1] of statistical solutions, which can be adopted when a semigroup of solution operators is not readily available. To be precise, for a given suitable initial Borel measure μ_0 supported on H, we construct in Section 4 an associated one-parameter family of measures $\{\mu_t\}_{t\geq 0}$ with the property that

$$\mu_t(E) = \lim_{k\to\infty} \sum_{j=1}^{N_k} \vartheta_{k,j}\delta_{S(t)\overline{Q}_{j,k}}(E)$$

for measurable subsets $E \subseteq H$, nematic profiles $\overline{Q}_{j,k} \in H$ and $t \geq 0$. One can then see each statistical solution $\{\mu_t\}_{t\geq 0} \in \mathcal{N}$ as a convenient concatenation of individual solutions $\{Q(\cdot,t)\}_{t\geq 0} \in \mathcal{M}$.

We store some more remarks on the construction of a phase portrait for the correlation function c_{μ_0} in the closing section 6.

1.4. **The Mathematical Model.** As we work with tensors, we consistently employ the Einstein summation convention over repeated lower indices. We now present a brief derivation of the models (1) and (2) introduced above.

In accordance with the Landau theory of phase transitions, the free energy density W is assumed to be a smooth map which is frame indifferent, in our case invariant under the action of the rotation group SO(3):

$$W\left(T_{\mathsf{R}}D, \mathsf{R}Q\mathsf{R}^T\right) = W\left(D, Q\right)$$

where $Q \in \mathrm{Sym}_0(3)$ and $(T_{\mathsf{R}}D)_{ijk} := \sum_{\ell,m,n=1}^{3} R_{i\ell}R_{jm}R_{kn}D_{\ell mn}$ for all $\mathsf{R} \in \mathrm{SO}(3)$ whenever D is a rank 3 tensor, i.e. W is hemitropic in its gradient argument and isotropic in its field argument. We assume that the corresponding free energy has the form

$$\int_{\mathbb{R}^3} W(\nabla Q(x), Q(x))\, dx = \int_{\mathbb{R}^3} \Big(E(\nabla Q(x)) + F(Q(x))\Big)\, dx$$

in which the elastic and bulk terms are decoupled. One may show by invariant theory that any such smooth isotropic map F is a smooth function $F_0 : \mathbb{R}\times\mathbb{R} \to \mathbb{R}$ of the principle invariants of SO(3)

$$\mathrm{tr}\left[Q^2\right] \qquad \text{and} \qquad \mathrm{tr}\left[Q^3\right].$$

We consider the energy functional

$$E_{\mathrm{LdG}}[Q] := \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla Q(x)|^2 + F_0(Q(x))\right)\, dx,$$

to which the elastic energy contribution is simply the Dirichlet energy, although one could work with more a general elastic energy of the form

$$\frac{L_1}{2}|\nabla Q|^2 + \frac{L_2}{2}\frac{\partial Q_{ik}}{\partial x_j}\frac{\partial Q_{ij}}{\partial x_k} + \frac{L_3}{2}\frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k} + \frac{L_4}{3}Q_{\ell k}\frac{\partial Q_{ik}}{\partial x_k}\frac{\partial Q_{ij}}{\partial x_\ell},$$

[1] See FOIAŞ ET AL. [8], Chapter V.

for $L_i > 0$, which is compatible with the system symmetry. We employ the simplest bulk energy density F_0 that is able to predict a first-order isotropic-nematic phase transition, namely

$$F_0(Q) := \frac{a(\theta)}{2}\mathrm{tr}\left[Q^2\right] - \frac{b}{3}\mathrm{tr}\left[Q^3\right] + \frac{c}{4}\left(\mathrm{tr}\left[Q^2\right]\right)^2, \tag{7}$$

where $a = a_0(\theta - \theta_c)$, $\theta_c > 0$ is the critical temperature and $\theta \in \mathbb{R}$ is a temperature parameter controlling the depths of the nematic energy wells. The material-dependent constants (a, b, c) belong to the bistable region

$$\mathcal{D} := \left\{(a,b,c) \in (0,\infty)^3 \, : \, b^2 > 27ac\right\}.$$

of parameter space $(0,\infty)^3$. The model for the dynamics of nematic liquid crystals we study is the L^2-gradient flow of the functional L_{LdG},

$$\frac{\partial Q}{\partial t} = \Delta Q - a(\theta)\, Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}\left[Q^2\right] I\right) - c\,\mathrm{tr}\left[Q^2\right] Q. \tag{8}$$

We consistently refer to (8) as the *Q-tensor equation*. Furthermore, we model the temperature quench as instantaneous, i.e. the parameters (a, b, c) lie in the bistable region $\mathcal{D}$ and do not depend on an evolving temperature field θ. Before the quench is effected at time $t = 0$, the parameters (a, b, c) lie in the complementary region $(0,\infty)^3 \setminus \mathcal{D}$: in this case, the isotropic phase $Q \equiv 0$ is a global minimiser of the bulk energy density (7) above.

We work over the whole space $\mathbb{R}^3$ so we need not worry about restricting the spatial domain of the correlation function (6). One may interpret this physically as modelling behaviour in the bulk of the nematic material, far from any boundaries where complicated boundary effects could come into play.

The main result of this paper is captured by the following statement.

STATEMENT OF MAIN RESULT. *For any given $\delta > 0$ there exist $\eta > 0$, depending only on δ and the parameters $(a, b, c) \in \mathcal{D}$, and an open dense subset*[2] *of*

$$\left\{R \in L^\infty(\mathbb{R}^3, \mathrm{Sym}_0(3)) \, : \, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1 + |x|)^{8+\delta} \, |R(x)| < \eta\right\},$$

such that for any Borel probability measure supported in this open dense set, the associated correlation function c_{μ_0} (6) *exhibits asymptotic self-similar behaviour, viz*

$$\left\| c_{\mu_0}(r,t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3,\, dr)} = \mathcal{O}\left(t^{-\frac{1}{2}}\right) \quad \textit{as} \quad t \to \infty.$$

1.5. **Structure of the Paper.** In SECTION 2, we record some preliminary results which allow us to establish a decomposition formula for 'small initial data' solutions of the Q-tensor equation in SECTION 3. The main result of the paper lies in SECTION 4, in which we establish asymptotic self-similarity of the correlation function c_{μ_0} by means of the previously-established decomposition formula. In the final section of the paper, we briefly discuss scaling behaviour of the correlation function corresponding to a class of

[2]The structure of this open dense set is described in section 4.1.

solutions starting from 'large' initial data, which gives rise to a different scaling regime for the correlation function, namely $L(t) = t$.

1.6. **Notation.** For any matrix $A \in \mathrm{Sym}_0(3)$ we denote its Frobenius norm by $|A| := \sqrt{A : A}$, where $A : B \equiv A_{ij}B_{ji}$ for $A, B \in \mathrm{Sym}_0(3)$. In what follows, unless otherwise stated, all Lebesgue spaces have range in $\mathrm{Sym}_0(3)$ and we write $L^p(\mathbb{R}^3, \mathrm{Sym}_0(3))$ simply as $L^p(\mathbb{R}^3)$ for $1 \le p \le \infty$. We also work with the phase space $H := L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$ endowed with the norm $\|Q\| := \max\{\|Q\|_2, \|Q\|_6\}$, where the norms $\|\cdot\|_p$ are given by

$$\|Q\|_p := \begin{cases} \left(\displaystyle\int_{\mathbb{R}^3} \left(\mathrm{tr}\left[Q(x)^2\right]\right)^{\frac{p}{2}}\, dx\right)^{\frac{1}{p}} & \text{when} \quad 1 \le p < \infty, \\ \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} |Q(x)| & \text{when} \quad p = \infty. \end{cases}$$

We denote the fundamental solution of the heat equation on $\mathbb{R}^3$ by Φ, namely

$$\Phi(x,t) := \frac{e^{-|x|^2/4t}}{(4\pi t)^{\frac{3}{2}}},$$

and denote the time-shifted profile $\Phi(x, t+1)$ simply by $\Phi_1(x,t)$. Finally, for any given $\delta > 0$ we denote by $\mathcal{A}$ the space of essentially bounded functions given by

$$\mathcal{A} := \left\{ Q \in L^\infty(\mathbb{R}^3) \;:\; \operatorname*{ess\,sup}_{x\in\mathbb{R}^3}\, (1+|x|)^{8+\delta}\, |Q(x)| < \infty \right\},$$

and equip it with the natural norm $\|Q\|_{\mathcal{A}} := \operatorname{ess\,sup}_{x\in\mathbb{R}^3}(1+|x|)^{8+\delta}|Q(x)|$. The constant $\delta > 0$ is chosen arbitrarily but remains *fixed*.

2. **Some Preliminary Results**

We now establish some results which enable us to comment on the long-time behaviour of the correlation function concentrated on individual solutions of the Q-tensor equation, namely the asymptotic behaviour as $t \to \infty$ of the quantity

$$c(r,t) = \frac{\displaystyle\int_{\mathbb{R}^3} \mathrm{tr}\left[Q(x,t)Q(x+r,t)\right]\, dx}{\displaystyle\int_{\mathbb{R}^3} \mathrm{tr}\left[Q(x,t)^2\right]\, dx},$$

where the initial datum $Q_0 \in H$ is chosen appropriately. We begin by stating a simple result on the well-posedness of the Q-tensor equation in the phase space H.

PROPOSITION 2.1. *For each $Q_0 \in H$ there exists a unique global classically-smooth solution Q of the Q-tensor equation (8) on $\mathbb{R}^3 \times (0,\infty)$ satisfying $\|Q(\cdot,t)\| < \infty$ for all $t > 0$. Furthermore, the nonlinear semigroup of solution operators $S(t) : H \to H$ defined by*

$$S(t)Q_0 := \begin{cases} Q_0, & \textit{if} \quad t = 0 \\ Q(\cdot, t; Q_0) & \textit{if} \quad t > 0 \end{cases}$$

for any $Q_0 \in H$ is strongly continuous.

Proof. The nonlinear semigroup $\{S(t)\}_{t\geq 0}$ is constructed by standard techniques. See Pazy [17] for details. $\square$

It is our aim to investigate finer properties of 'small initial data' solutions of (8), namely we wish to demonstrate a decomposition result for solutions starting from initial data which are small in the $\|\cdot\|_{\mathcal{A}}$-norm. In order to achieve this, we first must examine the long-time behaviour of solutions of the heat equation in $L^p(\mathbb{R}^3)$.

2.1. **A Remark on the Heat Equation in $\mathbb{R}^d$.** Consider the heat equation

$$\frac{\partial u}{\partial t}(x,t) = \Delta u(x,t) \qquad (x,t) \in \mathbb{R}^d \times (0,\infty),$$

where $1 \leq p \leq \infty$, $d \geq 1$ is an integer. For given $L^q(\mathbb{R}^d)$ initial data, it possesses a classically smooth solution on $\mathbb{R}^d \times (0,\infty)$ and this solution $u(x,t)$ may be expressed as a convolution involving the d-dimensional heat kernel $\Phi_d(x,t)$,

$$u(x,t) = (\Phi_d(\cdot,t) * u_0)(x) = \int_{\mathbb{R}^d} \frac{e^{-|x-y|^2/4t}}{(4\pi t)^{d/2}} u_0(y)\, dy,$$

for $t > 0$. In order to obtain an estimate on the time decay of solutions in $L^p(\mathbb{R}^d)$, one can employ Young's inequality in the above to produce

$$\|u(\cdot,t)\|_p \leq \frac{C(r)}{t^{\frac{d}{2}(1-\frac{1}{r})}} \|u_0\|_q,$$

for all $t > 0$ and $1 + 1/p = 1/q + 1/r$. Thus, all solutions of the heat equation with $L^q(\mathbb{R}^d)$ initial data decay to zero *at least* with rate $t^{-d/2+d/2r}$ as $t \to \infty$. We show in what is to come that if we insist that the initial data of the heat equation are of *zero mean* i.e. $\int_{\mathbb{R}^d} u_0 = 0$ and possess some mild decay condition at infinity, then we may improve our estimate on the rate of decay of the corresponding solution to 0 in $L^p(\mathbb{R}^d)$ as $t \to \infty$.

We begin with an auxiliary pointwise estimate on solutions of the heat equation that will be of help to us in the following section, and may indeed be of independent interest. We consider only the case of the heat equation in $\mathbb{R}^3$ appropriate to our considerations. The methods used here may be extended without great effort to capture a similar result in $\mathbb{R}^d$ for arbitrary dimension $d \geq 1$.

Proposition 2.2. *For $u_0 \in \mathcal{A}$, consider the difference*

$$\overline{m}(x,t) := (e^{t\Delta}u_0)(x) - \Phi(x,t) \int_{\mathbb{R}^3} u_0(y)\, dy.$$

For any $\beta > 0$, the estimate

$$|\overline{m}(x,t)| \leq Ct^{-2} \left(1 + \frac{|x|}{\sqrt{8t}}\right)^{-\beta} \int_{\mathbb{R}^3} |y| \left(1 + \frac{|y|}{\sqrt{8t}}\right)^{\beta} |u_0(y)|\, dy, \tag{9}$$

holds for $x \in \mathbb{R}^3$, $t > 0$. The explicitly-computable constant $C > 0$ depends only on β.

Proof. Define the map $\sigma : [0, 2\pi) \times [0, \pi) \to \mathbb{S}^2$, a standard surface patch parameterisation on the unit sphere, to be

$$\sigma(\vartheta, \varphi) := (\cos\vartheta \sin\varphi, \sin\vartheta \sin\varphi, \cos\varphi)\,,$$

and define $U : [0, \infty) \times [0, 2\pi) \times [0, \pi) \to \mathbb{R}$ by

$$U(r, \vartheta, \varphi) := \int_r^\infty u_0(\rho\cos\vartheta\sin\varphi, \rho\sin\vartheta\sin\varphi, \rho\cos\varphi)\rho^2 \sin\varphi \, d\rho.$$

Now, by a change of co-ordinates and an application of integration by parts, we deduce that

$$\begin{aligned}
&(e^{t\Delta}u_0)(x) \\
= \;& \int_0^\pi \int_0^{2\pi} \int_0^\infty \frac{e^{-|x - r\sigma(\vartheta,\varphi)|^2/4t}}{(4\pi t)^{3/2}} u_0(r\sigma(\vartheta, \varphi)) r^2 \sin\varphi \, dr d\vartheta d\varphi \\
= \;& \int_{\mathbb{R}^3} \Phi(x - r\sigma, t) \frac{\partial}{\partial r} \left(-U(r, \vartheta, \varphi)\right) \, dr d\vartheta d\varphi \\
= \;& \Phi \int_0^\pi \int_0^{2\pi} U(0, \vartheta, \varphi) \, d\vartheta d\varphi + \int_{\mathbb{R}^3} \frac{\sigma \cdot (x - r\sigma)}{2t} \Phi(x - r\sigma, t) U(r, \vartheta, \varphi) \, dr d\vartheta d\varphi \\
= \;& \Phi \int_{\mathbb{R}^3} u_0(y) \, dy + \int_{\mathbb{R}^3} \frac{\sigma \cdot (x - r\sigma)}{2t} \Phi(x - r\sigma, t) U(r, \vartheta, \varphi) \, dr d\vartheta d\varphi.
\end{aligned}$$

Applying the elementary inequality $\sqrt{z}\exp(-z) \leq \exp(-z/2)$ for $z \geq 0$, we deduce from the above

$$\begin{aligned}
&(e^{t\Delta}u_0)(x) - \Phi(x, t) \int_{\mathbb{R}^3} u_0(y) \, dy \\
\leq \;& \frac{1}{(4\pi)^{3/2}} \frac{1}{t^2} \int_{\mathbb{R}^3} e^{-|x - r\sigma|^2/8t} \left(\int_r^\infty |u_0(\rho\sigma)|\rho^2 d\rho \right) \sin\varphi \, dr d\vartheta d\varphi \\
\leq \;& Ct^{-2} \int_{\mathbb{R}^3} \sup_{(\vartheta,\varphi)} \left(e^{-|x - r\sigma|^2/8t}\right) \left(\int_r^\infty |u_0(\rho\sigma)|\rho^2 d\rho \right) \sin\varphi \, dr d\vartheta d\varphi \\
= \;& Ct^{-2} \int_{\mathbb{R}^3} e^{-(|x| - r)^2/8t} \left(\int_r^\infty |u_0(\rho\sigma)|\rho^2 d\rho \right) \sin\varphi \, dr d\vartheta d\varphi,
\end{aligned}$$

where $C > 0$ is independent of $t > 0$. A couple of applications of Fubini's theorem then yield

$$\begin{aligned}
\overline{m}(x, t) &\leq Ct^{-2} \int_0^\infty e^{-(|x| - r)^2/8t} \int_{|y| \geq r} |u_0(y)| \, dy \, dr \\
&= Ct^{-2} \int_{\mathbb{R}^3} \left(\int_0^\infty (1 - \chi_{B(0,r)}(y)) e^{-(|x| - r)^2/8t} \, dr \right) |u_0(y)| \, dy,
\end{aligned}$$

where $\chi_{B(0,r)}$ denotes the characteristic function of the open ball $B(0, r) \subset \mathbb{R}^3$. From this we find

$$\overline{m}(x, t) \leq Ct^{-2} \int_{\mathbb{R}^3} \left(\int_0^{|y|} e^{-(|x| - r)^2/8t} \, dr \right) |u_0(y)| \, dy. \tag{10}$$

We pause at this point to obtain a helpful estimate on the y-integrand in the above.

LEMMA 2.3. *For any $\beta > 0$, there exists a constant $C = C(\beta) > 0$ such that*

$$\int_{X-Y}^{X} e^{-\xi^2} d\xi \leq CY \left(\frac{1+Y}{1+X}\right)^{\beta} \quad \text{for } X, Y \geq 0. \tag{11}$$

Proof of Lemma. In what follows we fix $Y \geq 0$, considering it as a parameter. We separate the demonstration of the inequality into two cases.
(i) *The case where* $0 \leq X \leq Y$: One may easily deduce from the chain $0 \leq X \leq Y$ the simple inequality

$$Y \leq Y \left(\frac{1+Y}{1+X}\right)^{\beta},$$

for any $\beta > 0$. Using this, we have

$$\int_{X-Y}^{X} e^{-\xi^2}\, d\xi \leq \int_{X-Y}^{X} \max_{\xi_0} \left(e^{-\xi_0^2}\right) d\xi = Y \leq Y \left(\frac{1+Y}{1+X}\right)^{\beta}.$$

Thus, the claimed inequality holds for $0 \leq X \leq Y$.
(ii) *The case where* $Y \leq X$: This time, we have the estimate

$$\int_{X-Y}^{X} e^{-\xi^2}\, d\xi \leq \int_{X-Y}^{X} \sup_{\xi_0} \left(e^{-\xi_0^2}\right) d\xi = Y e^{-(X-Y)^2}.$$

Now, since there exists a constant $C > 1$ dependent only on $\beta > 0$ such that

$$e^{-Z^2} \leq C \left(\frac{1}{1+Z}\right)^{\beta},$$

for all $Z \geq 0$, and noting that

$$\left(\frac{1}{1+Z}\right)^{\beta} \leq \left(\frac{1+Y}{1+Y+Z}\right)^{\beta},$$

for all $Y \geq 0$, it follows from the substitution $Z \mapsto X - Y$ that

$$e^{-(X-Y)^2} \leq C \left(\frac{1+Y}{1+X}\right)^{\beta}.$$

for all $X \geq Y$. This estimate together with the first case estimate yields the result (11) above. □

We now return to the estimate (10) and close the proof of the proposition. Transforming the y-integrand through a simple change of variables provides

$$\begin{aligned}
\overline{m}(x,t) &\leq Ct^{-2} \int_{\mathbb{R}^3} \left(\int_0^{|y|} e^{-(|x|-r)^2/8t}\, dr \right) |u_0(y)|\, dy \\
&= Ct^{-2} \int_{\mathbb{R}^3} \left(\sqrt{8t} \int_{\frac{|x|}{\sqrt{8t}} - \frac{|y|}{\sqrt{8t}}}^{\frac{|x|}{\sqrt{8t}}} e^{-\xi^2}\, d\xi \right) |u_0(y)|\, dy. \qquad (12)
\end{aligned}$$

Finally, setting $X := |x|/(8t)^{1/2}$ and $Y := |y|/(8t)^{1/2}$, we apply the above lemma to (12), from which estimate (9) follows. □

Remark 2.4. Raising both sides to the power p and integrating over the domain $\mathbb{R}^3$, we may use the result in (9) to show that

$$\left\| e^{t\Delta} u_0 - \Phi(\cdot, t) \int_{\mathbb{R}^3} u_0(y)\, dy \right\|_p \leq \frac{C(p,\beta)}{t^{2-\frac{3}{2p}}} \int_{\mathbb{R}^3} |u_0(y)|(1+|y|)^{\beta+1}\, dy,$$

for $t > 0$. Therefore, if the initial data of the heat equation are of mean zero and lie in $L^1(\mathbb{R}^3; d\omega_\beta)$, where $d\omega_\beta := (1+|x|)^{\beta+1}dx$, we have improved upon the standard estimate obtained by Young's inequality for the time decay of solutions in $L^p(\mathbb{R}^3)$. Estimates of type (9) are key to obtaining a decomposition formula in the following section for solutions of (8). Let us also remark that the above result leads to a generalisation to higher spatial dimension of the work of TASKINEN [20].

3. A Decomposition Formula

We establish here a helpful structural formula for solutions of the Q-tensor equation starting from 'small' initial data. In particular, we show that the leading order asymptotics (up to order $t^{-3/2}$ in time after rescaling) of such solutions in all L^p-norms are governed by a matrix multiple of the heat kernel. It proves important in our subsequent analysis to consider a transformed version of the Q-tensor equation (8). If we set $R(x,t) := e^{at}Q(x,t)$ and substitute R into (8) in a formal manner, we obtain the equation

$$\partial_t R = \Delta R + b\, e^{-at}\left(R^2 - \frac{1}{3}\mathrm{tr}\left[R^2\right]\right) - c\, e^{-2at}\mathrm{tr}\left[R^2\right] R, \tag{13}$$

which is the principle equation of analysis in the section to come.

Let X_0 denote the set of maps

$$X_0 := \left\{ W \in C(\mathbb{R}^3 \times [0,\infty); \mathrm{Sym}_0(3)) \,\middle|\, \sup_{(x,t)} \omega(x,t)|W(x,t)| < \infty \right\},$$

where the space-time weight ω is defined to be

$$\omega(x,t) := \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}} (t+1)^2.$$

When endowed with the natural norm

$$\|W\|_{X_0} := \sup_{(x,t)} \omega(x,t)|W(x,t)|,$$

one may verify that X_0 admits the structure of a Banach space. We also employ the product space $X := \mathrm{Sym}_0(3) \times X_0$ furnished with the norm $\|\cdot\|_X := |\cdot| + \|\cdot\|_{X_0}$.

Remark 3.1. The space of maps X_0 with which we work from now on might seem at first glance rather ungainly. However, this space is only auxiliary in the sense that it does not feature in the hypotheses of THEOREM 3.1 below. In our setting, it is essentially the 'right' space in which to capture the first correction to the leading heat kernel asymptotics of small initial datum solutions of the transformed equation (13).

The main result of this section is contained in the following theorem.

THEOREM 3.1. *There exists $\eta > 0$ depending only on $(a,b,c) \in \mathcal{D}$ such that for initial data $Q_0 \in \mathcal{A} \subset H$ satisfying the smallness condition*

$$\|Q_0\|_{\mathcal{A}} \leq \eta, \tag{14}$$

the Q-tensor equation (8) *has a unique classically-smooth solution on* $\mathbb{R}^3 \times (0,\infty)$ *of the form*

$$Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t), \tag{15}$$

where $A \in \mathrm{Sym}_0(3)$ *and* $V \in X_0$.

3.1. **An Auxiliary System of Integral Equations.** With the above-defined Banach spaces in mind, for any given initial data $Q_0 \in \mathcal{A}$ consider the following nonlinear operator $F : X \to X$ associated with Q_0 defined componentwise as $F_1 : X \to \mathrm{Sym}_0(3)$, where

$$F_1(A,V) := \int_{\mathbb{R}^3} Q_0(y)\,dy + \int_0^\infty \int_{\mathbb{R}^3} h(A\Phi_1(y,s) + V(y,s), s)\,dyds, \tag{16}$$

and $F_2 : X \to X_0$, where

$$\begin{aligned} F_2(A,V;\cdot,t) \quad := \quad & e^{t\Delta}\left(Q_0 - \frac{e^{-|\cdot|^2/4}}{(4\pi)^{3/2}}\int_{\mathbb{R}^3} Q_0(y)\,dy\right) + \int_0^t e^{(t-s)\Delta}h(A\Phi_1(*,s) + V(*,s),s)\,ds \\ & - \Phi_1(\cdot,t)\int_0^\infty \int_{\mathbb{R}^3} h(A\Phi_1(y,s) + V(y,s),s)\,dyds. \end{aligned} \tag{17}$$

The function h is the nonlinearity in the transformed Q-tensor equation (13), and is given by

$$h(R,t) := b\,e^{-at}\left(R^2 - \frac{1}{3}\mathrm{tr}\left[R^2\right] I\right) - c\,e^{-2at}\mathrm{tr}\left[R^2\right] R,$$

for $R \in \mathrm{Sym}_0(3)$ and $t \geq 0$.

Suppose that there exists a fixed point (A^*, V^*) of the operator F in X, i.e. that the integral equations

$$A^* = F_1(A^*,V^*) \quad \text{and} \quad V^* = F_2(A^*,V^*)$$

hold in $\mathrm{Sym}_0(3)$ and X_0, respectively. Multiplying throughout the first equality above by $\Phi_1(x,t)$ and then adding the contribution of the second equality, one finds that the integral equation

$$A^*\Phi_1(\cdot,t) + V^*(\cdot,t) = e^{t\Delta}Q_0 + \int_0^t e^{(t-s)\Delta}h(A^*\Phi_1 + V^*, s)\,ds$$

holds for the assumed fixed point (A^*, V^*). Writing $R^* := A^*\Phi_1 + V^*$, we note that the above integral equation implies that R^* is classically smooth and satisfies (13) on $\mathbb{R}^3 \times (0,\infty)$. Following the time-dependent transformation effected by $Q^*(x,t) = e^{-at}R^*(x,t)$, one immediately finds that Q^* satisfies (8) on the same space-time domain. In turn, we may deduce from Proposition 2.1 (uniqueness of solutions) that for the chosen initial datum $Q_0 \in \mathcal{A} \subset H$, the corresponding solution Q^* of the Q-tensor equation admits the decomposition

$$Q^*(x,t) = A^*e^{-at}\Phi_1(x,t) + e^{-at}V^*(x,t),$$

for $t > 0$ as claimed. Therefore, in order to achieve this representation formula it suffices to show that the operator $F : X \to X$ possesses a fixed point in X for given $Q_0 \in \mathcal{A}$. We achieve this for a special class of Q_0 (namely those which satisfy $\|Q_0\|_{\mathcal{A}} < \eta$ for $\eta > 0$ sufficiently small) through an application of Banach's fixed point theorem. Establishing

the fact that F is locally Lipschitz on X is a little delicate, and we consider details of this calculation below.

3.2. **The Operator $F : X \to X$ is Locally Lipschitz.** In order to make our presentation more concise, we adopt the following notation. For given $A, B \in \mathrm{Sym}_0(3)$ and $V, W \in X_0$, we define the *contraction modulus* $k_0 \equiv k_0(A, B; V, W)$ to be

$$k_0 := (|A| + |B| + \|V\|_{X_0} + \|W\|_{X_0}) + (|A| + |B| + \|V\|_{X_0} + \|W\|_{X_0})^2 ,$$

and write $\phi \lesssim \psi$ whenever $\phi \leq Ck_0\psi$ and $C > 0$ is some absolute constant.[3] We demonstrate that the operator F satisfies the difference property

$$\|F(A, V) - F(B, W)\|_X \lesssim \|(A, V) - (B, W)\|_X,$$

for any $A, B \in \mathrm{Sym}_0(3)$ and $V, W \in X_0$, following which we deduce that F is indeed well-defined as an operator on and with range in X and thus is locally Lipschitz on X. Indeed, we gather these goals together in the following proposition.

Proposition 3.2. *The operator F associated with $Q_0 \in \mathcal{A}$ defined on X component-wise in (16) and (17) is well defined, i.e. has range in X, and also satisfies the local Lipschitz condition*

$$\|F(A, V) - F(B, W)\|_X \lesssim \|(A, V) - (B, W)\|_X, \tag{18}$$

whenever (A, V) and (B, W) belong to some bounded subset of X.

Proof. We begin by stating a useful estimate upon which we call frequently during the course of our proof.

Lemma 3.3. *For $A, B \in \mathrm{Sym}_0(3)$, $V, W \in X_0$, $x \in \mathbb{R}^3$ and $t \geq 0$, we have*

$$\begin{aligned} &|h(A\Phi_1(x, t) + V(x, t), t) - h(B\Phi_1(x, t) + W(x, t), t)| \\ \lesssim\ &\left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta} e^{-at}(t + 1)^{-3}\|(A, V) - (B, W)\|_X. \end{aligned} \tag{19}$$

We now look to obtain estimates on the components of F and its differences in the appropriate spaces.

3.2.1. *The component $F_1 : X \to \mathrm{Sym}_0(3)$.* The treatment of F_1 is straightforward: following an application of the estimate (19), we deduce that the inequality

$$|F_1(A, V) - F_1(B, W)| \leq C_1 k_0(A, B; V, W)\|(A, V) - (B, W)\|_X \tag{20}$$

holds for any $A, B \in \mathrm{Sym}_0(3)$ and $V, W \in X_0$ and constant $C_1 > 0$. Furthermore, one can quickly verify that $\mathrm{tr}[F_1(A, V)] = 0$ and indeed $F_1(A, V) < \infty$ for any $(A, V) \in X$.

We now turn our attention to the component F_2, whose analysis requires considerably more care than that of F_1. It proves to be prudent to cleave our estimates into

[3] To avoid any confusion which may arise from line to line, we interpret the string $\phi \lesssim \psi \lesssim \omega$ as $\phi \leq C_1 k_0 \psi \leq C_2 k_0 \omega$.

one part which is in a neighbourhood of the origin in time, and one other part which is bounded away from zero in time. We now consider the more involved case when time t is bounded away from the origin.

3.2.2. *The component* $F_2 : X \to X_0$ *when* $t \geq 1$. A judicious splitting of integrals faciliates a swift analysis. For $(A,V),(B,W) \in X$, we begin by writing the difference as

$$F_2(A,V;x,t) - F_2(B,V;x,t) = I(x,t) + J(x,t),$$

where

$$I(\cdot,t) := \int_{t/2}^{t} e^{(t-s)\Delta}\big(h(A\Phi_1 + V, s) - h(B\Phi_1 + W, s)\big)\, ds,$$

and

$$\begin{aligned} J(\cdot,t) := \quad & \int_0^{t/2} e^{(t-s)\Delta}\big(h(A\Phi_1 + V, s) - h(B\Phi_1 + W, s)\big)\, ds \\ & - \Phi_1(\cdot,t)\int_0^\infty \int_{\mathbb{R}^3} \big(h(A\Phi_1(y,\tau) + V(y,\tau),\tau) - h(B\Phi_1(y,\tau) + W(y,\tau),\tau)\big)\, dyd\tau. \end{aligned}$$

We deal initially with the estimate on the term I and consider its temporal integrand, given by

$$\int_{\mathbb{R}^3} \frac{e^{-|x-y|^2/4(t-s)}}{(4\pi(t-s))^{3/2}} \left(h(A\Phi_1(y,s) + V(y,s),s) - h(B\Phi_1(y,s) + W(y,s),s)\right)\, dy. \tag{21}$$

for $x \in \mathbb{R}^3$, $t \geq 1$ and $t/2 \leq s \leq t$. For any given fixed $x \in \mathbb{R}^3$ the inequality

$$\left(1 + \frac{|y|}{\sqrt{s+1}}\right)^{-8-\delta} \leq C\left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta} \tag{22}$$

holds for all $\delta > 0$, $t/2 \leq s \leq t$ and y in the region $\mathcal{R}_1(x)$, where

$$\mathcal{R}_1(x) := \left\{ y \in \mathbb{R}^3 \,:\, |x-y| \leq \frac{|x|}{2} \right\},$$

and the constant $C > 0$ depends only on $\delta > 0$. For this given $x \in \mathbb{R}^3$, we consider the integral (21) but over the region $\mathcal{R}_1(x)$ as opposed to the whole space:

$$\begin{aligned} & \int_{\mathcal{R}_1(x)} \Phi(x-y,t-s)\left(h(A\Phi_1 + V,s) - h(B\Phi_1 + W,s)\right)\, ds \\ & \overset{(19)}{\lesssim} \frac{\|(A,V) - (B,W))\|_X}{e^{as}(s+1)^3} \int_{\mathcal{R}_1(x)} \Phi(x-y,t-s)\left(1 + \frac{|y|}{\sqrt{s+1}}\right)^{-8-\delta} dy \\ & \overset{(22)}{\lesssim} \frac{\|(A,V) - (B,W))\|_X}{e^{as}(s+1)^3} \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta} \int_{\mathcal{R}_1(x)} \Phi(x-y,t-s)\, dy \\ & \lesssim \frac{\|(A,V) - (B,W))\|_X}{e^{as}(s+1)^3} \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{-8-\delta}. \end{aligned} \tag{23}$$

For the same fixed $x \in \mathbb{R}^3$, the inequality

$$\exp\left(-\frac{1}{8}\frac{|x-y|^2}{(t-s)}\right) \leq C\left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} \tag{24}$$

holds for y in the region $\mathcal{R}_2(x) := \mathbb{R}^3 \setminus \mathcal{R}_1(x)$, whenever $t/2 \le s \le t$. Now proceeding in a similar manner as we did for the region $\mathcal{R}_1(x)$, we find that

$$\begin{aligned}
&\int_{\mathcal{R}_2(x)} \Phi(x-y,t-s)\left(h(A\Phi_1(y,s)+V(y,s),s) - h(B\Phi_1(y,s)+W(y,s),s)\right)\,dy \\
&= \int_{\mathcal{R}_2(x)} \frac{e^{-|x-y|^2/8(t-s)}}{(4\pi(t-s))^{3/2}} e^{-|x-y|^2/8(t-s)}\left(h(A\Phi_1+V,s)-h(B\Phi_1+W,s)\right)\,dy \\
&\overset{(24)}{\le} C\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} \int_{\mathcal{R}_2(x)} \frac{e^{-|x-y|^2/8(t-s)}}{(4\pi(t-s))^{3/2}} \left|h(A\Phi_1+V,s)-h(B\Phi_1+W,s)\right|\,dy \\
&\overset{(19)}{\lesssim} \frac{\|(A,V)-(B,W))\|_X}{e^{as}(s+1)^3}\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} \int_{\mathcal{R}_2(x)} \frac{e^{-|x-y|^2/8(t-s)}}{(4\pi(t-s))^{3/2}}\,dy.
\end{aligned} \tag{25}$$

Combining results (23) and (25) we obtain

$$\begin{aligned}
&\int_{\mathbb{R}^3} \Phi(x-y,t-s)\left(h(A\Phi_1(y,s)+V(y,s),s) - h(B\Phi_1(y,s)+W(y,s),s)\right)\,dy \\
&\lesssim \frac{1}{e^{as}(s+1)^3}\left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} \|(A,V)-(B,W))\|_X.
\end{aligned} \tag{26}$$

Finally, integrating (26) with respect to s over the interval $t/2 \le s \le t$, we find

$$I(x,t) \lesssim \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2}\|(A,V)-(B,W)\|_X, \tag{27}$$

as desired. Let us progress to the required estimate for J.

It is at this point we utilise the heat equation 'decay improvement' Proposition 2.2. For convenience, for our chosen $(A,V),(B,W) \in X$ we denote by $h_0 : \mathbb{R}^3 \times (0,\infty) \to \mathrm{Sym}_0(3)$ the map

$$h_0(x,t) := h(A\Phi_1(x,t)+V(x,t),t) - h(B\Phi_1(x,t)+W(x,t),t).$$

If we denote by $\overline{M}(x,t,s)$ the quantity

$$\overline{M}(\cdot,t,s) := \int_{\mathbb{R}^3} \frac{e^{-|\cdot-y|^2/4(t-s)}}{(4\pi(t-s))^{3/2}} h_0(y,s)\,dy - \Phi(\cdot,t-s)\left(\int_{\mathbb{R}^3} h_0(y,s)\,dy\right)$$

and also stipulate that $H_0 : (0,\infty) \to \mathrm{Sym}_0(3)$ be

$$H_0(t) := \int_t^\infty \int_{\mathbb{R}^3} h_0(y,\tau)\,dyd\tau,$$

one may verify that the identity

$$\begin{aligned}
J(x,t) = &\overbrace{\int_0^{t/2} \overline{M}(x,t,s)\,ds}^{J_1(x,t):=} + \overbrace{H_0(0)\big(\Phi(x,t)-\Phi_1(x,t)\big)}^{J_2(x,t):=} - \overbrace{\Phi\left(x,\frac{t}{2}\right)H_0\left(\frac{t}{2}\right)}^{J_3(x,t):=} \\
&+ \underbrace{\int_0^{t/2}\left(\frac{6\pi}{t-s} - \frac{|x|^2}{4(t-s)^2}\right)\Phi(x,t-s)H_0(s)\,ds}_{J_4(x,t):=}
\end{aligned} \tag{28}$$

holds for all $x \in \mathbb{R}^3$ and $t \ge 1$. It is straightforward to show that

$$J_i(x,t) \lesssim \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2}\|(A,V)-(B,W)\|_X, \tag{29}$$

for $i = 3, 4$ simply by using familiar properties of the heat kernel, inequality (19) and the fact that $(t-s)^{-1} \leq 4(t+1)^{-1}$ for $t \geq 1$ and s in the interval $0 \leq s \leq t/2$. The treatment of the cases $i = 1, 2$ require a little more care. An application of the result of Proposition 2.2 to the term J_1 yields

$$\begin{aligned}
&\int_0^{t/2} \overline{M}(x,t,s)\, ds \\
\overset{(9)}{\leq}\ & C \int_0^{t/2} \int_{\mathbb{R}^3} \frac{|y|}{(t-s)^2} \left(\frac{1 + |y|/\sqrt{8(t-s)}}{1 + |x|/\sqrt{8(t-s)}} \right)^{4+\frac{\delta}{2}} |h(A\Phi_1 + V, s) - h(B\Phi_1 + W, s)|\ dyds, \\
\overset{(19)}{\lesssim}\ & \int_0^{t/2} \frac{e^{-as}}{(s+1)^3} \int_{\mathbb{R}^3} \frac{|y|}{(t-s)^2} \left(1 + \frac{|y|}{\sqrt{8(t-s)}} \right)^{4+\frac{\delta}{2}} \left(1 + \frac{|y|}{\sqrt{s+1}} \right)^{-8-\delta} dyds \\
& \times \left(1 + \frac{|x|}{\sqrt{8(t-s)}} \right)^{-4-\frac{\delta}{2}} \|(A,V) - (B,W))\|_X.
\end{aligned}$$

Now, noticing that for $0 \leq s \leq t/2$ and $t \geq 1$ we have the string of inequalities $(t-s)^{-1/2} \leq \sqrt{2} t^{-1/2} \leq C(t+1)^{-1/2} \leq C(s+1)^{-1/2}$, we deduce from the above that

$$\begin{aligned}
&\int_0^{t/2} \overline{M}(x,t,s)\, ds \\
\lesssim\ & \int_0^{t/2} \left(1 + \frac{|x|}{\sqrt{8(t-s)}} \right)^{-4-\frac{\delta}{2}} \frac{e^{-as}}{(s+1)} \frac{1}{(t-s)^2} \left(\int_{\mathbb{R}^3} (1+|y|)^{-3-\frac{\delta}{2}}\, dy \right) ds \\
& \times \|(A,V) - (B,W))\|_X \\
\lesssim\ & \left(1 + \frac{|x|}{\sqrt{t+1}} \right)^{-4-\frac{\delta}{2}} (t+1)^{-2} \|(A,V) - (B,W))\|_X, \qquad (30)
\end{aligned}$$

since $\delta > 0$ gives us the required integrability of $(1 + |\cdot|)^{-3-\delta/2}$ in dimension three. It remains to verify such an estimate holds for the term J_2, and for this we require the following simple lemma.

Lemma 3.4. *For $x \in \mathbb{R}^3$ and $t \geq 1$, the heat kernel difference $\Phi_1(x,t) - \Phi(x,t)$ satisfies the inequality*

$$|\Phi_1(x,t) - \Phi(x,t)| \leq \frac{2e^{-|x|^2/8(t+1)}}{(t+1)^{5/2}}. \qquad (31)$$

Proof of Lemma. Consider the smooth map ψ defined by

$$\psi(z,t) := e^{-\frac{z^2}{4}\left(\frac{1}{2(t+1)}\right)} - e^{-\frac{z^2}{4}\left(\frac{2+t}{2t(t+1)}\right)}.$$

For any fixed $t \geq 1$, by considering the equation $\psi_z(z,t) = 0$ one may show that $z \mapsto \psi(z,t)$ is controlled by its unique global maximum over the set $[1, \infty)$, namely

$$\psi(z,t) \leq 2 \left(\frac{1}{\frac{2}{t} + 1} \right)^{t/2} \frac{1}{t+1}.$$

Upon setting $z = |x|^2$, we readily deduce from the above

$$e^{-|x|^2/4(t+1)} - e^{-|x|^2/4t} \leq \frac{2e^{-|x|^2/8(t+1)}}{(t+1)},$$

from which estimate (31) quickly follows. $\square$

Piecing this together with the estimates (29) and (30), we obtain

$$J(x,t) \lesssim \|(A,V)-(B,W)\|_X \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2},$$

which along with (27) provides

$$|F_2(A,V;x,t) - F_2(B,W;x,t)| \lesssim \|(A,V)-(B,W)\|_X \left(1+\frac{|x|}{\sqrt{t+1}}\right)^{-4-\frac{\delta}{2}} (t+1)^{-2}, \tag{32}$$

for $x \in \mathbb{R}^3$ and $t \geq 1$.

3.2.3. *The component $F_2 : X \to X_0$ when $0 \leq t \leq 1$.* This case follows almost immediately from (19) and the fact that our time interval of interest in this instance is compact. Thus, combining this with (32), rearranging and taking norms in X_0, we find that

$$\|F_2(A,V) - F_2(B,W)\|_{X_0} \leq C_2 k_0(A,B;V,W)\|(A,V)-(B,W)\|_X \tag{33}$$

for some constant $C_2 > 0$. We have therefore verified the difference property (18).

3.2.4. *The operator $F_2 : X \to X_0$ is well defined.* All that remains to be checked is that the map

$$(x,t) \mapsto \int_{\mathbb{R}^3} \frac{e^{-|x-y|^2/4t}}{(4\pi t)^{3/2}} \left(Q_0(y) - \frac{e^{-|y|^2/4}}{(4\pi)^{3/2}} \int_{\mathbb{R}^3} Q_0(z)\, dz\right) dy$$

is an element of X_0. The case when $t \geq 1$ may be tackled using inequality (9) and Lemma 3.4. On the other hand, for the case when $0 \leq t \leq 1$, we need only concern ourselves with the behaviour of the heat term $e^{t\Delta}Q_0$ near the origin in time. We obtain the required estimates by writing

$$(e^{t\Delta}Q_0)(x) = \int_{\mathcal{R}_1(x)} \Phi(x-y,t)Q_0(y)\, dy + \int_{\mathcal{R}_2(x)} \Phi(x-y,t)Q_0(y)\, dy$$

and applying inequalities (22) and (24) in the manner previously outlined over the regions $\mathcal{R}_1(x)$ and $\mathcal{R}_2(x)$, respectively.

Finally, setting $(B,W) = 0$ in (33) completes the proof that $F : X \to X$ is both well-defined and locally Lipschitz on X. $\square$

Let $\mathfrak{B} := \overline{B(0,\varepsilon_0)} \subset X$ denote the closed ball of radius $\varepsilon_0 > 0$ in X, where ε_0 is yet to be fixed. To close the proof of Theorem 3.1 by means of an application of Banach's fixed point theorem, it remains to show that $F : \mathfrak{B} \to \mathfrak{B}$ is a strictly contractive operator for ε_0 chosen sufficiently small. To this end, fix ε_0 to be the positive root of the quadratic equation associated with the contraction constraint

$$\max\{C_1, C_2\}\left(2\varepsilon + 4\varepsilon^2\right) = \frac{1}{4},$$

and taking into account the definition of the contraction modulus k_0, we deduce from (20) and (33) that

$$\|F(A,V) - F(B,W)\|_X \leq \frac{1}{2}\|(A,V) - (B,W)\|_X,$$

for all $(A,V),(B,W) \in \mathfrak{B}$. Given that we also have the estimate

$$\begin{aligned}\|F(A,V)\|_X \leq \quad & \sup_{(x,t)} \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}} (t+1)^2 \left| e^{t\Delta}\left(Q_0 - \frac{e^{-|\cdot|^2/4}}{(4\pi)^{3/2}}\int_{\mathbb{R}^3} Q_0(z)\,dz\right)(x)\right| \\ & + \left|\int_{\mathbb{R}^3} Q_0(y)\,dy\right| + \frac{1}{2}\|(A,V)\|_X,\end{aligned}$$

for any $(A,V) \in \mathfrak{B}$, it is clear we may find $\eta > 0$ to ensure that the quantity

$$\sup_{(x,t)} \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}} (t+1)^2 \left| e^{t\Delta}\left(Q_0 - \frac{e^{-|\cdot|^2/4}}{(4\pi)^{3/2}}\int_{\mathbb{R}^3} Q_0(z)\,dz\right)(x)\right| + \left|\int_{\mathbb{R}^3} Q_0(y)\,dy\right|$$

is less than or equal to $\varepsilon_0/2$ for all $Q_0 \in \mathcal{A}$ satisfying $\|Q_0\|_{\mathcal{A}} \leq \eta$. Thus, for all such Q_0 satisfying this 'smallness' condition, the associated nonlinear operators F are strictly contractive with range in $\mathfrak{B}$. By the Banach fixed point theorem, there exists a unique (relabeled) fixed point $(A,V) \in X$ and so from the discussion in section 3.1 follows the proof of Theorem 3.1, namely

$$Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t),$$

for some $A \in \mathrm{Sym}_0(3)$ and $V \in X_0$ satisfying $\|(A,V)\|_X \leq \varepsilon_0$.

Remark 3.2. We henceforth denote by $\mathcal{A}^\circ$ the open subset of all initial data $Q_0 \in \mathcal{A}$ for which the above decomposition result holds, namely

$$\mathcal{A}^\circ := \left\{ R \in L^\infty(\mathbb{R}^3) \;:\; \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1+|x|)^{8+\delta}\,|R(x)| < \eta \right\}. \tag{34}$$

4. The Scaling Regime $L(t) = t^{1/2}$

Before we discuss the behaviour of the correlation function $c_{\mu_0}(r,t)$ as $t \to \infty$, we comment on the behaviour of the correlation function concentrated on *individual* solutions. Utilising the decomposition formula $Q(x,t) = Ae^{-at}\Phi_1(x,t) + e^{-at}V(x,t)$ obtained in Theorem 3.1, we investigate how the quantity

$$c(r,t) = \frac{\int_{\mathbb{R}^3} \mathrm{tr}\left[Q(x+r,t)Q(x,t)\right]\,dx}{\int_{\mathbb{R}^3} \mathrm{tr}\left[Q(x,t)^2\right]\,dx}$$

behaves for large time. Firstly, noting that we have the equality

$$\int_{\mathbb{R}^3} \Phi_1(x+r,t)\Phi_1(x,t)\,dx = \frac{1}{\sqrt{8}}\frac{e^{-|r|^2/8(t+1)}}{(4\pi(t+1))^{3/2}},$$

and also that any $V \in X_0$ has the norm decay property

$$\|V(\cdot,t)\|_2 \leq C\|V\|_{X_0}(t+1)^{-5/4},$$

one may then verify that

$$\frac{\sqrt{8}e^{2at}(4\pi(t+1))^{3/2}}{\operatorname{tr}[A^2]}\int_{\mathbb{R}^3}\operatorname{tr}\left[Q(x+r,t)Q(x,t)\right]\,dx \le e^{-|r|^2/8(t+1)}+\omega(t), \tag{35}$$

for $r\in\mathbb{R}^3$ *provided* $A\neq 0$, where the function ω is bounded and continuous on $[1,\infty)$ and decays at least as quickly at $t^{-1/2}$ as $t\to\infty$. Setting $r=0$ in (35) above and taking the appropriate quotient, one quickly finds that

$$c(r,t)-e^{-|r|^2/8t}\le\frac{1}{1+\omega(t)}\left(e^{-|r|^2/8(t+1)}-e^{-|r|^2/8t}\right)-\frac{\omega(t)}{1+\omega(t)}e^{-|r|^2/8t}+\frac{\omega(t)}{1+\omega(t)},$$

from which we deduce

$$\left\|c(r,t)-e^{-\frac{|r|^2}{8t}}\right\|_{L^\infty(\mathbb{R}^3;\,dr)}=\mathcal{O}\left(t^{-1/2}\right)\quad\text{as}\quad t\longrightarrow\infty. \tag{36}$$

Let us reiterate that the above calculation is only valid whenever the constant matrix A is non-zero. If $A=0$, one discovers

$$c(r,t)=\frac{\displaystyle\int_{\mathbb{R}^3}\operatorname{tr}\left[V(x+r,t)V(x,t)\right]\,dx}{\displaystyle\int_{\mathbb{R}^3}\operatorname{tr}\left[V(x,t)^2\right]\,dx},$$

from which no scaling information on the correlation function can be gleaned. This is not the case when $A\neq 0$, as the map $(r,t)\mapsto e^{-|r|^2/8t}$ is manifestly self-similar on $\mathbb{R}^3\times(0,\infty)$. We now demonstrate that the set of all initial data in $\mathcal{A}^\circ$ which possibly give rise to solutions for which $A=0$ in the decomposition (15) is rare.

4.1. **The matrix A cannot be zero on 'large' sets of initial data in $\mathcal{A}^\circ$.** It is our aim to show that the scaling behaviour of solutions is generic amongst all those evolving from initial data satisfying the smallness condition (14). Our notion of 'generic' here is that the set of all such initial data in $\mathcal{A}^\circ$ giving rise to solutions with constant matrix $A=0$ constitute a closed set containing no open ball.

Firstly, let us note that as each $Q_0\in\mathcal{A}^\circ$ has a corresponding unique solution of the shape

$$Q(x,t)=Ae^{-at}\Phi_1(x,t)+e^{-at}V(x,t), \tag{37}$$

and each matrix A satisfies the explicit identity (c.f. formula (16))

$$A=\int_{\mathbb{R}^3}Q_0(y)\,dy+\int_0^\infty\int_{\mathbb{R}^3}h(Q(y,\tau),\tau)\,dyd\tau,$$

we can ask about the nature of the resulting map between $\mathcal{A}^\circ$ and $\mathrm{Sym}_0(3)$ which yields A from Q_0. It is well known that real-analytic maps between open connected sets of Banach spaces cannot be constant on open subsets unless they are identically constant on the whole set. Thus, if we demonstrate the map $Q_0\mapsto A$ is real-analytic on $\mathcal{A}^\circ$ and is indeed not identically the zero map, it follows that the set of all such initial data which produce the result $A=0$ in the decomposition (37) is rare: more precisely, it is closed in $\mathcal{A}^\circ$ and contains no open ball.

In this direction, consider the map $\mathcal{F}_0 : \mathcal{X} \times \mathcal{A} \to \mathcal{X}$ defined by

$$\mathcal{F}_0(Z(\cdot,t),z) := e^{t\Delta} z + \int_0^t e^{(t-s)\Delta} h(Z(\cdot,s),s)\, ds - Z(\cdot,t),$$

for $Z \in \mathcal{X}$, $z \in \mathcal{A}$ and $t \geq 0$, where $\mathcal{X}$ is the Banach space of maps

$$\mathcal{X} := \left\{ U \in C(\mathbb{R}^3 \times [0,\infty); \mathrm{Sym}_0(3)) \, : \, \sup_{(x,t)} \left(1 + \frac{|x|}{\sqrt{t+1}}\right)^{4+\frac{\delta}{2}} (t+1)^{3/2} |U(x,t)| < \infty \right\}$$

endowed with the natural weighted supremum norm $\|\cdot\|_{\mathcal{X}}$. We also recall that the space $\mathcal{A}$ is endowed with the norm $\|R\|_{\mathcal{A}} = \mathrm{ess\,sup}_{x\in\mathbb{R}^3}(1+|x|)^{8+\delta}|R(x)|$. In what follows, we wield results from the theory of analytic Banach space-valued maps. We refer the reader to Zeidler [22] for the basic definitions and results. As a helpful first step, we establish the following proposition.

Proposition 4.1. *The map $\mathcal{F}_0 : \mathcal{X} \times \mathcal{A} \to \mathcal{X}$ is real-analytic.*

Proof. By considering the difference

$$\mathcal{F}_0[(R,\rho) + (\Xi,\xi)] - \mathcal{F}_0[(R,\rho)],$$

one may check that the first Fréchet derivative $d\mathcal{F}_0$ of $\mathcal{F}_0$ at $(R,\rho) \in \mathcal{X} \times \mathcal{A}$ satisfies

$$\begin{aligned}(d\mathcal{F}_0[(R,\rho)])(\Xi,\xi) &= e^{t\Delta}\xi + b\int_0^t e^{(t-s)\Delta} e^{-as}\left(R\Xi + \Xi R - \frac{2}{3}\mathrm{tr}\,[R\Xi]\, I\right) ds \\ &\quad - c\int_0^t e^{(t-s)\Delta} e^{-2as}\left(2\,\mathrm{tr}\,[R\Xi]\, R + \mathrm{tr}\left[R^2\right]\Xi\right) ds - \Xi(\cdot,t), \qquad (38)\end{aligned}$$

for all $(\Xi,\xi) \in \mathcal{X} \times \mathcal{A}$. Owing to the fact that the nonlinearity h in the operator $\mathcal{F}_0$ is of cubic order, the higher Fréchet derivatives satisfy

$$\left(d^k\mathcal{F}[(R,\rho)]\right)((\Xi_1,\xi_1),...,(\Xi_k,\xi_k)) = 0 \quad \text{in} \quad \mathcal{X},$$

for $(R,\rho), (\Xi_1,\xi_1)..., (\Xi_k,\xi_k) \in \mathcal{X} \times \mathcal{A}$ and $k \geq 4$. Furthermore, for constants C, K and r depending on the point (R,ρ), the estimates

$$\|d^k\mathcal{F}_0[(Z,z)]\| \leq \frac{Ck!}{K^k}, \quad \text{whenever} \quad \|(Z,z) - (R,\rho)\|_{\mathcal{X}\times\mathcal{A}} < r$$

hold for $0 \leq k < 4$, where norms are taken in the appropriate space of multilinear operators. By triviality of the higher Fréchet derivatives, the map $\mathcal{F}_0$ is real-analytic on $\mathcal{X} \times \mathcal{A}$. $\square$

This result aids us in establishing the useful fact that the solution map $\mathcal{F} : Q_0 \mapsto Q$ from $\mathcal{A}^\circ$ to $\mathcal{X}$ is itself a real-analytic map.

Theorem 4.2. *The solution map $\mathcal{F} : \mathcal{A}^\circ \to \mathcal{X}$ is real-analytic.*

Proof. In what follows, we call $(R,\rho) \in \mathcal{X} \times \mathcal{A}$ a *solution pair* if and only if $R \in \mathcal{X}$ is the unique solution of (13) corresponding to the initial datum $\rho \in \mathcal{A}$. We denote the corresponding *solution map* which yields R from ρ by $\mathcal{F}$. We make the important observation that for any point $(R,\rho) \in \mathcal{X} \times \mathcal{A}$,

$$\mathcal{F}_0[(R,\rho)] = 0 \qquad \text{if and only if} \qquad (R,\rho) \text{ is a solution pair.} \qquad (39)$$

Suppose (R,ρ) chosen from the open subset $\mathcal{X}\times\mathcal{A}^\circ\subset\mathcal{X}\times\mathcal{A}$ is a solution pair. We claim that the partial derivative $d_Z\mathcal{F}_0[(R,\rho)]\in\mathcal{L}(\mathcal{X})$ is a homeomorphism.

As the partial Fréchet derivative $d_Z\mathcal{F}_0$ satisfies

$$\begin{aligned}(d_Z\mathcal{F}_0[(R,\rho)])(\Xi) &= b\int_0^t e^{(t-s)\Delta}e^{-as}\left(R\Xi+\Xi R-\frac{2}{3}\mathrm{tr}\,[R\Xi]\,I\right)ds\\ &-c\int_0^t e^{(t-s)\Delta}e^{-2as}\left(2\,\mathrm{tr}\,[R\Xi]\,R+\mathrm{tr}\left[R^2\right]\Xi\right)ds-\Xi(\cdot,t).\end{aligned}$$

for all $\Xi\in\mathcal{X}$, one may then verify that the inequality

$$\|d_Z\mathcal{F}_0[(R,\rho)]-J\|_{L(\mathcal{X})}<1$$

holds by 'smallness' in the $\|\cdot\|_{\mathcal{X}}$-norm of those solutions of (13) starting from $\mathcal{A}^\circ$ initial data. Furthermore, the map $J:\mathcal{X}\to\mathcal{X}$ given by $J\Xi:=-\Xi$ clearly has unit norm in $\mathcal{L}(\mathcal{X})$. It then follows from the theory of Neumann series that $d_Z\mathcal{F}_0[(R,\rho)]\in L(\mathcal{X})$ is a homeomorphism. Thus, by the analytic implicit function theorem, one may infer the existence of an open neighbourhood $\mathcal{V}\subset\mathcal{A}^\circ$ of ρ, an open neighbourhood $\mathcal{U}\subset\mathcal{X}\times\mathcal{A}^\circ$ of the point (R,ρ) and a real-analytic map $\phi:\mathcal{V}\to\mathcal{X}$ with the property that

$$\{(\phi(\rho),\rho)\;:\;\rho\in\mathcal{V}\}=\mathcal{F}_0^{-1}(0)\cap\mathcal{U}.$$

By observation (39), it is clear that the set $\mathcal{F}_0^{-1}(0)$ is simply that of all solution pairs $(\mathcal{F}\rho,\rho)$ such that $\rho\in\mathcal{A}$. Therefore, the map $\phi:\mathcal{V}\to\mathcal{X}$ is identically equal to the restriction $\mathcal{F}|_{\mathcal{V}}$ of the solution operator to the set $\mathcal{V}\subset\mathcal{A}^\circ$.

As the point (R,ρ) was arbitrarily chosen, it then follows that the solution operator $\mathcal{F}:\mathcal{A}^\circ\to\mathcal{X}$ is real-analytic. □

By virtue of this theorem, it is clear that the map $\rho\mapsto(R,\rho)$ sending an initial datum $\rho\in\mathcal{A}^\circ$ to its solution pair is real-analytic on $\mathcal{A}^\circ$. By a routine calculation, one may also verify that the map

$$(Z,z)\mapsto\int_{\mathbb{R}^3}z(y)\,dy+\int_0^\infty\int_{\mathbb{R}^3}h(Z(y,\tau),\tau)\,dyd\tau$$

from $\mathcal{X}\times\mathcal{A}^\circ$ to $\mathrm{Sym}_0(3)$ is also real analytic. With these facts in mind, one may view the right-hand side of the equality

$$A=\int_{\mathbb{R}^3}Q_0(y)\,dy+\int_0^\infty\int_{\mathbb{R}^3}h(Q(y,\tau),\tau)\,dyd\tau$$

as a composition of analytic maps taking $\mathcal{X}\times\mathcal{A}^\circ$ to $\mathrm{Sym}_0(3)$. As compositions of real analytic maps are themselves real analytic, we deduce that the map $Q_0\mapsto A$ is real analytic on $\mathcal{A}^\circ$.

We need only now show that this map is non-zero on $\mathcal{A}^\circ$. To this end, we provide a non-empty set of initial data contained in $\mathcal{A}^\circ$ for which the matrix A in the decomposition (15) is non-zero. Together with the fact that the coefficient matrix A depends in a continuous manner on initial data, we have the existence of an open set of initial data for which $A\neq 0$.

PROPOSITION 4.3. *For $\alpha \geq 0$, let $\lambda_\alpha : \mathbb{R}^3 \to \mathbb{R}$ denote the map*

$$\lambda_\alpha(x) := -\frac{\alpha}{(1+|x|)^{8+\delta}}. \tag{40}$$

If $Q_{0,\alpha} := \mathrm{diag}(\lambda_\alpha, \lambda_\alpha, -2\lambda_\alpha)$, then there exists $\alpha_0 > 0$ such that $A \neq 0$ in the decomposition (15) for all $0 < \alpha < \alpha_0$.

Proof. By uniqueness of solutions of (8), it follows that solutions remain of the form $Q(x,t) = \mathrm{diag}(\lambda(x,t), \lambda(x,t), -2\lambda(x,t))$ for $t > 0$, where $\lambda(x,t)$ satisfies the nonlinear heat equation

$$\frac{\partial \lambda}{\partial t} = \Delta\lambda - a\,\lambda - b\,\lambda^2 - 6c\,\lambda^3$$

on $\mathbb{R}^3 \times (0,\infty)$. By THEOREM 3.1, we are ensured of an $\varepsilon > 0$ such that

$$|\lambda(x,t)| \leq C\varepsilon \quad \text{on} \quad \mathbb{R}^3 \times (0,\infty),$$

for some constant $C > 0$ depending only on $(a,b,c) \in \mathcal{D}$.

Now, setting $\mu(x,t) := e^{at}\lambda(x,t)$, for $\alpha_0 > 0$ chosen small enough we have

$$-b\,e^{-at}\,(\mu(x,t))^2 - c\,e^{-2at}\,(\mu(x,t))^3 \leq 0 \quad \text{on} \quad \mathbb{R}^3 \times (0,\infty).$$

Furthermore, since μ satisfies the equation

$$\mu(\cdot,t) = e^{t\Delta}\lambda_0 - \int_0^t e^{(t-s)\Delta}\left(b\,e^{-as}\,(\mu(\cdot,s))^2 + 6c\,e^{-2as}\,(\mu(\cdot,s))^3\right)ds,$$

by integrating across over space, we deduce

$$\int_{\mathbb{R}^3} \mu(x,t)\,dx \leq \int_{\mathbb{R}^3} \lambda_0(x,t)\,dx < 0.$$

Thus, the $L^1(\mathbb{R}^3)$-norm of the solution cannot decay to 0 as $t \to \infty$, and so for the set of initial data

$$\left\{\mathrm{diag}(\lambda_0,\lambda_0,-2\lambda_0) \,:\, \lambda_0(x) = -\frac{\alpha}{(1+|x|)^{8+\delta}} \quad \text{for} \quad 0 < \alpha < \alpha_0\right\} \subset \mathcal{A}^\circ,$$

the corresponding matrix A in the solution decomposition (15) cannot be zero. $\square$

From this we conclude that the map $Q_0 \mapsto A$ is not identically the zero map on $\mathcal{A}^\circ$. It follows that the set of all those Q_0 in $\mathcal{A}^\circ$ which yield $A = 0$ in (37) is closed and contains no open ball.

Remark 4.1. We subsequently denote the set of all points in $\mathcal{A}^\circ$, for which we do not have information on the coefficient matrix A by $\mathcal{B}$.

4.2. **Asymptotic Behaviour of $c_{\mu_0}(r,t)$ as $t \to \infty$.** As discussed in the introduction, we express the notion of averaging over initial conditions in a rigorous manner by evaluating the correlation function with respect to a suitable time-dependent family of Borel probability measures. We construct statistical solutions of (8) in the following proposition, whose proof is a modification of a construction contained in FOIAS, MANLEY, ROSA AND TEMAM [8]. We quickly recall the definition a Dirac delta measure on the space $L^2(\mathbb{R}^3)$.

Definition 4.1. For any given $Q \in L^2(\mathbb{R}^3)$, the associated map $\delta_Q : \mathcal{P}(L^2(\mathbb{R}^3)) \to \{0,1\}$ defined by

$$\delta_Q(A) := \begin{cases} 1 & \text{if} \quad Q \in A, \\ \\ 0 & \text{otherwise,} \end{cases}$$

is the *Dirac delta measure* concentrated at $Q \in L^2(\mathbb{R}^3)$.

PROPOSITION 4.4. *Suppose* $0 < \gamma < \infty$. *For any given Borel probability measure* $\overline{\mu}$ *supported on the set*

$$\left\{Q \in L^2(\mathbb{R}^3) \,:\, \|Q\|_2 \leq \gamma\right\} \cap H,$$

there exists a one-parameter family of Borel probability measures $\{\mu_t\}_{t\geq 0}$ *satisfying*

$$\mu_t(E) = \lim_{k\to\infty} \sum_{j=1}^{N_k} \vartheta_{k,j}\delta_{S(t)\overline{Q}_{k,j}}(E), \tag{41}$$

for all measurable subsets $E \subseteq K$ *and* $t \geq 0$. *For each* $k \geq 1$, *the coefficients* $\vartheta_{k,j} \geq 0$ *respect the sum* $\sum_j \vartheta_{k,j} = 1$, *and* $S(t)\overline{Q}_{k,j}$ *denotes the action of the semigroup of* PROPOSITION 2.1 *on initial data* $\overline{Q}_{k,j}$.

Proof. We establish the spaces which we use to construct the family of measures $\{\mu_t\}_{t\geq 0}$. We endow the set

$$K := \left\{Q \in L^2(\mathbb{R}^3) \,:\, \|Q\|_2 \leq \gamma\right\}$$

with the weak topology inherited from $L^2(\mathbb{R}^3)$, with respect to which it is a compact topological space. Furthermore, this space is metrizable with metric d_w, given by

$$d_w(Q,R) := \sum_{k=1}^{\infty} \frac{1}{2^k} \left| \int_{\mathbb{R}^3} Q : \chi_k - \int_{\mathbb{R}^3} R : \chi_k \right|,$$

where $\{\chi_k\}_{k=1}^{\infty}$ is a countable dense subset of the set $K \subset L^2(\mathbb{R}^3)$. We write $\mathsf{M}_0(K)$ to denote the set of all Borel probability measures carried by subsets of K, and furnish $\mathsf{M}_0(K)$ with the subspace weak-$*$ topology inherited from $C(K)'$, whence $\mathsf{M}_0(K)$ is itself a convex, compact Hausdorff topological space by the Banach-Alaoglu theorem. We make the observation from the estimate

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^3} \mathrm{tr}\left[Q^2\right] \leq \left(\frac{b^2}{2c} - a\right)\int_{\mathbb{R}^3} \mathrm{tr}\left[Q^2\right],$$

which may be derived from (8), that there exists $T = T(Q_0, \gamma) > 0$ such that the solution $Q(\cdot, t)$ satisfies

$$Q(\cdot, t) \in \left\{R \in L^2(\mathbb{R}^3) \,:\, \|R\|_2 \leq \gamma\right\},$$

for all $0 \leq t \leq T$ whenever $Q(\cdot, 0) = Q_0 \in K \cap H$. Furthermore, we write σ_T to denote the set of solution trajectories

$$\sigma_T := \{Q \in C([0,T], K) \,:\, Q(x,t) \;\text{ solves }\; (8) \;\text{ and }\; Q(\cdot,0) \in K \cap H\} \subset C([0,T]; K).$$

Using suitable properties of solutions of the Q-tensor equation (8), by the Arzelà-Ascoli theorem σ_T is itself a compact topological space with respect to the topology induced from $C([0,T];K)$, where

$$d_\infty(Q_1,Q_2) := \max_{0\le t\le T} d_w(Q_1(t),Q_2(t)).$$

Similarly, the space $\mathsf{M}_0(\sigma_T)$ is also a convex, compact Hausdorff topological space.

Let us now begin our construction. For a given $\overline{\mu} \in \mathsf{M}_0(K)$ supported on $K\cap H$, by the Krein-Milman theorem we know there exists a sequence of families of Dirac delta measures $\{\delta_{\overline{Q}_{k,j}}\}_{j=1}^{N_k}$ for $k = 1,2,3,...$ satisfying

$$\int_K \varphi\, d\overline{\mu} = \lim_{k\to\infty} \sum_{j=1}^{N_k} \vartheta_{k,j} \int_K \varphi\, d\delta_{\overline{Q}_{k,j}} \quad \text{for all} \quad \varphi \in C(K).$$

Using this approximating sequence of measures, we define a new sequence of probability measures $\{\mu^k\}_{k=1}^\infty \subset \mathsf{M}_0(\sigma_T)$ by

$$\mu^k := \sum_{j=1}^{N_k} \vartheta_{k,j} \delta_{Q(\cdot\,;\overline{Q}_{k,j})},$$

where $Q(\cdot\,;\overline{Q}_{k,j})$ denotes the solution trajectory starting from the initial datum $\overline{Q}_{k,j}$. This defines a sequence of points in $\mathsf{M}_0(\sigma_T)$, so by compactness there exists a measure $\mu \in \mathsf{M}_0(\sigma_T)$ to which a (relabeled) subsequence of $\{\mu^k\}_{k=1}^\infty$ converges in the weak-$*$ topology. We now focus on this limiting measure μ.

For each fixed $s \in [0,T]$, the map

$$\varphi \mapsto \int_{\sigma_T} \varphi(Q(s))\, d\mu$$

is well defined, positive and linear on $C(K)$, so by the Riesz-Kakutani theorem there exists a Borel probability measure μ_s (depending on the choice of $s \in [0,T]$) satisfying

$$\int_{\sigma_T} \varphi(Q(s))\, d\mu(Q) = \int_K \varphi(R)\, d\mu_s(R)$$

for all $\varphi \in C(K)$. By direct computation, one may show for the sequence of approximants $\{\mu^k\}_{k=1}^\infty$ that the equality

$$\int_{\sigma_T} \varphi(Q(s))\, d\mu^k(Q) = \int_K \varphi(R)\, d\mu_s^k(R)$$

holds for all $\varphi \in C(K)$, where

$$\mu_s^k := \sum_{j=1}^{N_k} \vartheta_{k,j} \delta_{S(s)\overline{Q}_{k,j}}.$$

Using the fact that $\mu^k \rightharpoonup \mu$ weakly-star in $\mathsf{M}_0(\sigma_T)$, we find

$$\int_K \varphi(R)\, d\mu_t = \int_{\sigma_T} \varphi(Q(t))\, d\mu(Q) = \lim_{k\to\infty} \int_{\sigma_T} \varphi(Q(t))\, d\mu^k = \lim_{k\to\infty} \int_K \varphi(R)\, d\mu_t^k(R).$$

From this we deduce the result

$$\mu_t(E) = \lim_{k\to\infty} \mu_t^k(E), \tag{42}$$

for all measurable subsets $E \subseteq K$. One completes the proof of the theorem by noting that $\lim_{t\to 0}\mu_t(E) = \mu_0(E)$ and that the transport of the measure μ_0 may be extended globally in time as the semigroup $\{S(t)\}_{t\geq 0}$ is defined globally in time. $\square$

Assembling all that has come before, we now approach the proof of our main result, which follows rather swiftly from previous results.

THEOREM 4.5. *For any given $\delta > 0$, there exists $\eta > 0$ depending only on δ and the parameters $(a, b, c) \in \mathcal{D}$ such that for any Borel probability measure μ_0 supported in the open dense set*

$$\mathcal{A}^\circ \setminus \mathcal{B} = \left\{ R \in L^\infty(\mathbb{R}^3) \,:\, \operatorname*{ess\,sup}_{x\in\mathbb{R}^3} (1+|x|)^{8+\delta} \, |R(x)| < \eta \right\} \setminus \mathcal{B},$$

the associated correlation function (6) *exhibits asymptotic self-similar behaviour*:

$$\left\| c_{\mu_0}(r,t) - e^{-\frac{|r|^2}{8t}} \right\|_{L^\infty(\mathbb{R}^3,\,dr)} = \mathcal{O}(t^{-1/2}) \quad \textit{as} \quad t \to \infty.$$

Proof. By the previous result (41), we know that

$$\sum_{j=1}^{N_k} \vartheta_j^k \delta_{S(t)\overline{Q}_{k,j}}(E) \to \mu_t(E)$$

as $k \to \infty$ for any measurable subset $E \subset \mathcal{A}^\circ \setminus \mathcal{B}$. Since we have that

$$c_{\mu_0}(r,t) = \lim_{k\to\infty} \frac{\displaystyle\sum_{j=1}^{N_k} \vartheta_{k,j} \int_H \int_{\mathbb{R}^3} \operatorname{tr}\left[Q(x+r)Q(x)\right]\, dx d\delta_{S(t)\overline{Q}_{k,j}}(Q)}{\displaystyle\sum_{j=1}^{N_k} \vartheta_{k,j} \int_H \int_{\mathbb{R}^3} \operatorname{tr}\left[Q(x)^2\right]\, dx d\delta_{S(t)\overline{Q}_{k,j}}(Q)}.$$

the result then follows by employing the same calculation as was used to achieve (36). $\square$

5. The Scaling Regime $L(t) = t$: An Observation

We now present evidence to support the existence of another scaling regime for the correlation function c_{μ_0}, namely $L(t) = t$, when μ_0 is concentrated on initial profiles whose $L^2(\mathbb{R}^3)$-norm is *not* restricted in magnitude in the manner of THEOREM 3.1.

Suppose that we offer initial data $Q_0 \in H$ of the form $Q_0 = \operatorname{diag}(\lambda_0, \lambda_0, -2\lambda_0)$ for equation (8). By uniqueness (PROPOSITION 2.1) we know the solution Q remains of diagonal form $Q = \operatorname{diag}(\lambda, \lambda, -2\lambda)$, where λ satisfies the *scalar* nonlinear heat equation

$$\frac{\partial \lambda}{\partial t} = \Delta\lambda - a\,\lambda - b\,\lambda^2 - 6c\,\lambda^3. \tag{43}$$

For any $R > 0$ we denote by $\lambda_{0,R} : \mathbb{R}^3 \to \mathbb{R}$ the map

$$\lambda_{0,R}(x) := \begin{cases} \lambda^* & \text{if} \quad |x| < R, \\ 0 & \text{otherwise}, \end{cases}$$

where λ^* is the global minimiser of the bulk potential associated with (43), namely

$$\lambda^* = \min_{\lambda\in\mathbb{R}} \left(\frac{a}{2}\lambda^2 + \frac{b}{3}\lambda^3 + \frac{3c}{2}\lambda^4\right).$$

In order to comment on the asymptotic behaviour of the correlation function concentrated on such solutions, we require the following result (which we state without proof) that is based on the observations of Aronson and Weinberger [1] and Poláčik [18] that equation (43) supports *pulse-like* solutions.

Proposition 5.1. *There exist $R_0 > 0$ and $\overline{c} > 0$ such that solutions of* (43) *subject to initial data $\lambda_{0,R}$ for $R \geq R_0$ satisfy*

$$\lim_{t\to\infty} \|\lambda(\cdot,t) - \lambda^*\|_{L^\infty(B(0,\overline{c}t))} = 0, \tag{44}$$

where $B(0,\overline{c}t) \subset \mathbb{R}^3$ denotes the ball of radius $\overline{c}t$ and centre 0. Furthermore, for any $t_0 > 0$ there exists $\vartheta = \vartheta(t_0)$ such that the solution λ satisfies the bounds

$$0 \leq \lambda(x,t) \leq Ce^{-\sigma(|x|-\overline{c}t+\vartheta)} \quad \text{on} \quad \mathbb{R}^3 \times [t_0,\infty), \tag{45}$$

for some positive constants C and σ.

Utilising the results (44) and (45) above, one may verify that the correlation function

$$c_{\delta_{Q_0}}(r,t) = \frac{\displaystyle\int_{\mathbb{R}^3} \lambda(x+r,t)\lambda(x,t)\,dx}{\displaystyle\int_{\mathbb{R}^3} \lambda(x,t)\lambda(x,t)\,dx}$$

concentrated on solutions with initial data $Q_0 = \operatorname{diag}(\lambda_{0,R}, \lambda_{0,R}, -2\lambda_{0,R})$ for $R \geq R_0$ satisfies

$$\lim_{t\to\infty} \left\| c_{\delta_{Q_0}}(r,t) - P\left(\frac{|r|}{t}\right)\right\|_{L^\infty(\mathbb{R}^3,\,dr)} = 0,$$

where P is a cubic polynomial of the shape

$$P(z) = \frac{1}{13\overline{c}^3}\,(4\overline{c}+z)\,(2\overline{c}-z)^2\,.$$

Thus, for this one-parameter family of initial data, whose H-norm may be made arbitrarily large, we obtain *both* a different universal scaling function (a polynomial, as opposed to the exponential map) and a different form for the coarsening length scale $L(t)$.

6. **Closing Remarks**

In this article, we have been able to obtain asymptotic information for $c_{\mu_0}(\cdot,t)$ in $L^\infty(\mathbb{R}^3)$ for μ_0 probing a rather restricted region of phase space H. Ideally, one would wish to be able to decompose phase space $H = \cup_{j\in J} H_j$ in such a manner that given the knowledge $\operatorname{supp}\mu_0 \subseteq H_i \subset H$, one could find non-trivial $\Gamma_i : \mathbb{R}^3 \to \mathbb{R}$ and $L_i : (0,\infty) \to (0,\infty)$ such that

$$\lim_{t\to\infty} \left\| c_{\mu_0}(r,t) - \Gamma_i\left(\frac{r}{L_i(t)}\right)\right\|_{L^\infty(\mathbb{R}^3,\,dr)} = 0.$$

It is in this sense we hope to find a *phase portrait* for c_{μ_0} defined on H from our earlier comments contained in the introduction.

Furthermore, our main result THEOREM 3.1 is a small initial data result which one would expect to hold for a wide class of reaction-diffusion equations, and in particular scalar equations. It is not clear whether or not the high-dimensional target space of the reaction-diffusion system (8) supports behaviour of c_{μ_0} distinct from that of correlation functions defined on scalar equations.

Finally, it would be of some interest to investigate how the influence of flow (governed by, say, a Navier-Stokes type system) might affect the form of the scaling function Γ or length-scale L. These are problems we hope to tackle in future work.

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